```
=> d his

     (FILE 'HOME' ENTERED AT 09:33:39 ON 23 APR 2004)

     FILE 'REGISTRY' ENTERED AT 09:34:59 ON 23 APR 2004
                E NORIBIGAINE/CN
L1            1 S E4

     FILE 'CAPLUS' ENTERED AT 09:36:48 ON 23 APR 2004
L2           54 S L1 OR HYDROXYIBOGAMINE OR NORIBOGAINE OR DEMETHYLIBOGAINE
L3            5 S L2 AND (PAIN OR ANALGE?)
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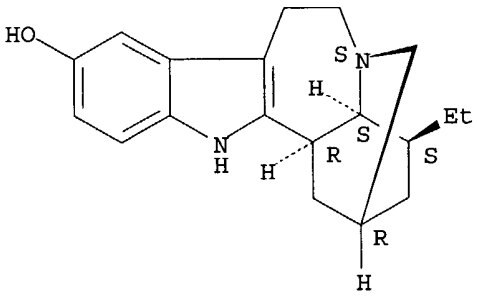
=> s e4
L1 1 NORIBOGAINE/CN

=> d rn str cn

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 481-88-9 REGISTRY

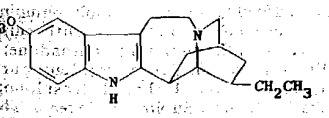
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

CN Ibogamin-12-ol (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 6,9-Methano-5H-pyrido[1',2':1,2]azepino[4,5-b]indole, ibogamin-12-ol deriv.
CN Ibogaine, O-demethyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN 12-Hydroxyibogamine
CN **Noribogaine**
CN O-Demethylibogaine
CN O-Noribogaine

4806. Ibogaine. *12-Methoxyibogamine.* $C_{20}H_{26}N_2O$; mol wt 310.42. C 77.38%, H 8.44%, N 9.03%, O 5.15%. Indole alkaloid of the *iboga* group. Isoln from root (1.27%), root-bark (2 to 6%), stems (1.95%) and leaves (0.35%) of the shrub *Tabernanthe iboga* Baill., *Apocynaceae*, found in Africa: Dybowski, Landrin, *Compt. Rend.* **133,** 748 (1901); Haller, Heckel, *ibid.* 850, 1236; from other *Apocynaceae:* H. Achenbach, B. Raffelsberger, *Z. Naturforsch.* **35B,** 219, 885 (1980); N. Ghorbel *et al., J. Nat. Prod.* **44,** 717 (1981); T. Mulamba *et al., ibid.* 184; B. Richard *et al., ibid.* **46,** 283 (1983). Purification: Schlittler *et al., Helv. Chim. Acta* **36,** 1941 (1953). Revised extraction procedure: Dickel *et al., J. Am. Chem. Soc.* **80,** 123 (1958). Review of early isolation work: Lebeau, Janot, *Traité de Pharmacie Chimique* **vol. 4** (Masson et Cie., Paris, 1956) pp 2982-2988. Structure: Bartlett *et al., J. Am. Chem. Soc.* **80,** 126 (1958). Mass spectrum: Biemann, Friedmann-Spiteller, *ibid.* **83,** 4805 (1961). Synthesis: Büchi *et al., ibid.* **88,** 3099 (1966); Rosenmund *et al., Ber.* **108,** 1871 (1975). Derivs: Taylor, U.S. pat. **2,877,229** (1959 to Ciba). Absolute configuration: K. Bláha *et al., Tetrahedron Letters* **1972,** 2763. Interatomic distances similar to those of serotonin: J. M. Kelley, R. H. Adamson, *Pharmacology* **10,** 28 (1973). NMR spectrum: E. Wenkert *et al., Helv. Chim. Acta* **59,** 2437 (1976). Determn in biological fluids: E. Bertol *et al., J. Chromatog.* **117,** 239 (1976). Iboga extracts said to be used by African natives while stalking game, to enable them to remain motionless for as long as 2 days while retaining mental alertness. Neuropharmacological studies: Schneider, Sigg, *Ann. N.Y. Acad. Sci.* **66,** 765 (1957); S. Gershon, W. J. Lang, *Arch. Int. Pharmacodyn. Ther.* **135,** 31 (1962). Cardiovascular effects: J. A. Schneider, R. K. Rinehart, *ibid.* **110,** 92 (1957). Serotonergic properties: R. S. Sloviter *et al., J. Pharmacol. Exp. Ther.* **214,** 231 (1980). Experimental use in treatment of heroin addiction: H. S. Lotsof, U.S. pat. **4,499,096** (1985). Review: W. I. Taylor, "The Iboga and Voacanga Alkaloids" in *The Alkaloids, Chemistry and Physiology* **Vol. 8,** R. H. F. Manske, Ed. (Academic Press, New York, 1965) p 203-235, *ibid.* **Vol. 11** (1968), pp 79-98.

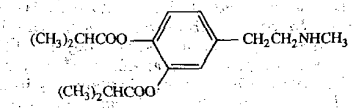


Prismatic needles from abs ethanol, mp 152-153°. Sublimes 150°. $[\alpha]_D^{20}$ −53° (in 95% ethanol). pKa 8.1 in 80% methylcellosolve. uv max (methanol): 226, 298 nm (log ε 4.93). Sol in ethanol, ether, chloroform, acetone, benzene. Practically insol in water.

Hydrochloride, $C_{20}H_{27}ClN_2O$, crystals. Dec 299-300°. $[\alpha]_D$ −63° (ethanol); $[\alpha]_D^{25}$ −49° (H_2O). Soluble in water, methanol, ethanol. Slightly sol in acetone, chloroform. Practically insol in ether.

CAUTION: This is a controlled substance (hallucinogen) listed in the U.S. Code of Federal Regulations, Title 21 Part 1308 (1985).

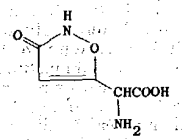
4807. Ibopamine. *2-Methylpropanoic acid 4-[2-(methylamino)ethyl]-1,2-phenylene ester;* 4-[2-(methylamino)ethyl]-1,2-phenylene diisobutyrate; *N*-methyldopamine diisobutyric acid di-*o*-isobutyryl epinine. $C_{17}H_{25}NO_4$; mol wt 307.39. C 66.42%, H 8.20%, N 4.56%, O 20.82%. Inotropic agent with dopaminergic and adrenergic agonist activities. Synth: G. Casagrande, G. Ferrari, Ger. pat. **2,734,678;** U.S. pat. **4,218,470** (1978, 1980 both to Simes). Pharmacology: G. F. Melloni *et al., Curr. Ther. Res.* **25,** 406 (1979); *ibid.* **26,** 466 (1979). Diuretic effect in chronic liver cirrhosis: S. Stefoni *et al., Brit. J. Clin. Pharmacol.* **11,** 69 (1981). In ascitic liver disease: G. F. Melloni *et al., ibid.* **12,** 71 (1981). Acute hemodynamic effects in congestive heart failure: G. Ghirardi *et al., ibid.* **19,** 613 (1985). α- and β-adrenergic activity: A. J. Nichols, R. R. Ruffolo, Jr., *J. Pharmacol. Exp. Ther.* **242,** 455 (1987). Series of articles on study: D. Sher, V. Ferrari, *ibid.* **37,** 869 (1987). Review of pharmacodynamics, pharmacokinetics and therapeutic efficacy: J. M. Henwood, P. A. Todd, *Drugs* **36,** 11-31 (1988).



Hydrochloride, $C_{17}H_{26}ClNO_4$, *SB 7505, Inopamil, Scandine.* Crystals from ethyl acetate, mp 132°.

THERAP CAT: Cardiotonic.

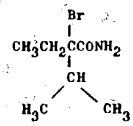
4808. Ibotenic Acid. *α-Amino-2,3-dihydro-3-oxo-5-isoxazoleacetic acid; α-amino-3-hydroxy-5-isoxazoleacetic acid;* amino-(3-hydroxy-5-isoxazolyl)acetic acid. $C_5H_6N_2O_4$; mol wt 158.11. C 37.98%, H 3.83%, N 17.71%, O 40.48%. Fly-killing and narcosis-potentiating amino acid structurally similar to kainic acid, *q.v.*, extracted from poisonous mushroom species. Isoln from *Amanita pantherina* (DC.) Fr., and *A. muscaria* (L.) Fr., *Agaricaceae:* Takemoto *et al., J. Pharm. Soc. Japan* **84,** 1233 (1964); Eugster *et al., Tetrahedron Letters* **1965,** 1813. Structure: Takemoto *et al., J. Pharm. Soc. Japan* **84,** 1186, 1232 (1964). Syntheses: Gagneux *et al., Tetrahedron Letters* **1965,** 2081; Sirakawa *et al., Chem. Pharm. Bull.* **14,** 89 (1966); Kishida *et al., ibid.* **14,** 92 (1966); **15,** 1025 (1967). Improved synthesis: Nakamura, *ibid.* **19,** 46 (1971). Industrial pats: **Belg. pat. 665,249,** *C.A.* **65,** 2266e (1966); Gagneux *et al.,* U.S. pat. **3,459,862** (1965, 1969, both to Geigy); Kishida *et al.,* **Japan.** pats. **15,975('68)** and **25,780('69)** (both to Sankyo), *C.A.* **70,** 77944p (1969); **72,** 13054g (1970). Pharmacology: Theobald *et al., Arzneimittel-Forsch.* **18,** 311 (1968); Johnston *et al., Biochem. Pharmacol.* **17,** 2488 (1968). Exhibits potent neuroexcitatory activity: *eidem, Nature* **248,** 804 (1974). Chemistry review: Eugster, *Fortschr. Chem. Org. Naturst.* **27,** 261-321 (1969); Catalfomo, Eugster, *Bull. Narcotics* **22,** 33-41 (1970). Excitatory and possible sedative actions on spinal neurons: D. R. Curtis *et al., J. Physiol.* **291,** 19 (1979); in cerebral cortex: E. Puil, *Can. J. Physiol. Pharmacol.* **59,** 1025 (1981). Use as experimental neurotoxic agent: A. Contestabile *et al., Experientia* **40,** 524 (1984).



Crystals from water or methanol, mp 151-152° (anhydrous); mp 144-146° (monohydrate). LD_{50} in mice, rats (mg/kg): 15, 42 i.v.; 38, 129 orally (Theobald).

USE: Neurobiological tool.

4809. Ibrotamide. *2-Bromo-2-ethyl-3-methylbutanamide;* α-bromo-α-isopropylbutyramide; α-ethyl-α-isopropyl-α-bromoacetamide; 2-bromo-2-ethylisovaleramide; Vagoprol. $C_7H_{14}BrNO$; mol wt 208.12. C 40.40%, H 6.78%, Br 38.40%, N 6.73%, O 7.69%. Prepn: Hildebrandt *et al.,* U.S. pat. **1,780,131** (1931 to Knoll); Safir *et al., J. Am. Chem. Soc.* **77,** 4840 (1955).



Crystals, mp 51°. Soluble in the usual organic solvents and in oil.

THERAP CAT: Sedative, hypnotic.

4810. Ibudilast. *2-Methyl-1-[2-(1-methylethyl)pyrazolo-*